



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 6RPU / pdb_00006rpu
Title : Structure of the ternary complex of the IMPDH enzyme from *Ashbya gossypii* bound to the dinucleoside polyphosphate Ap5G and GDP
Authors : Buey, R.M.; Fernandez-Justel, D.; Revuelta, J.L.
Deposited on : 2019-05-14
Resolution : 2.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

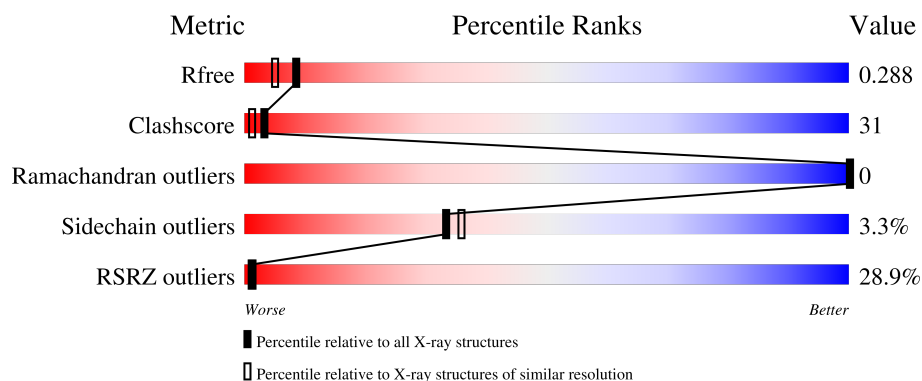
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	522	24% 50% 31% • 17%

2 Entry composition [i](#)

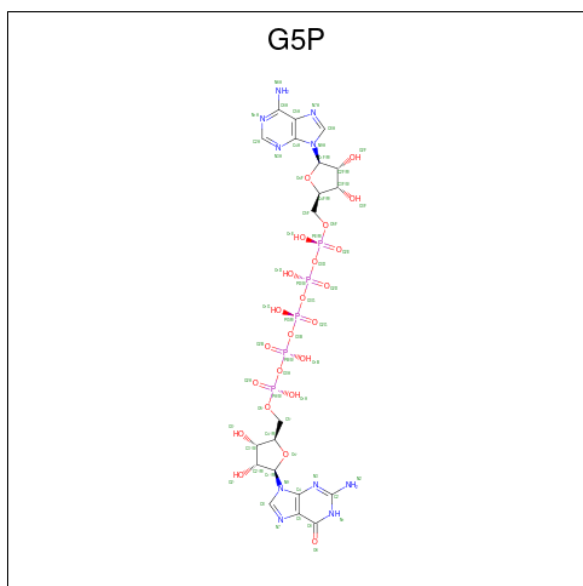
There are 5 unique types of molecules in this entry. The entry contains 6538 atoms, of which 3213 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	432	6336	2003	3165	547	599	22	0	0	0

- Molecule 2 is P1-(5'-ADENOSYL)-P5-(5'-GUANOSYL) PENTAPHOSPHATE (CCD ID: G5P) (formula: $C_{20}H_{29}N_{10}O_{23}P_5$) (labeled as "Ligand of Interest" by depositor).



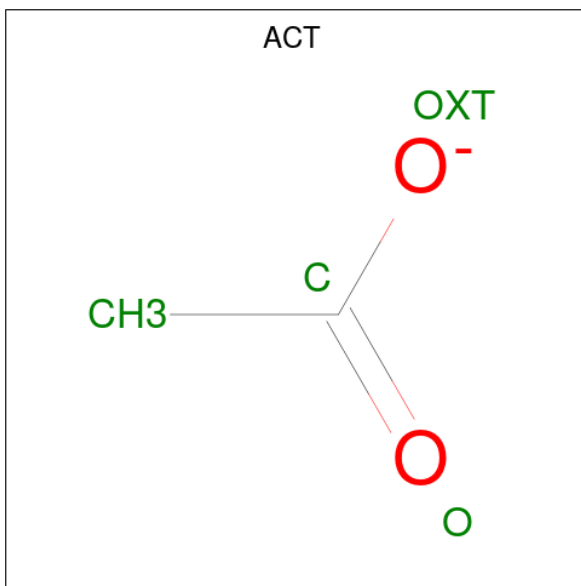
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	82	20	24	10	23	5	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		

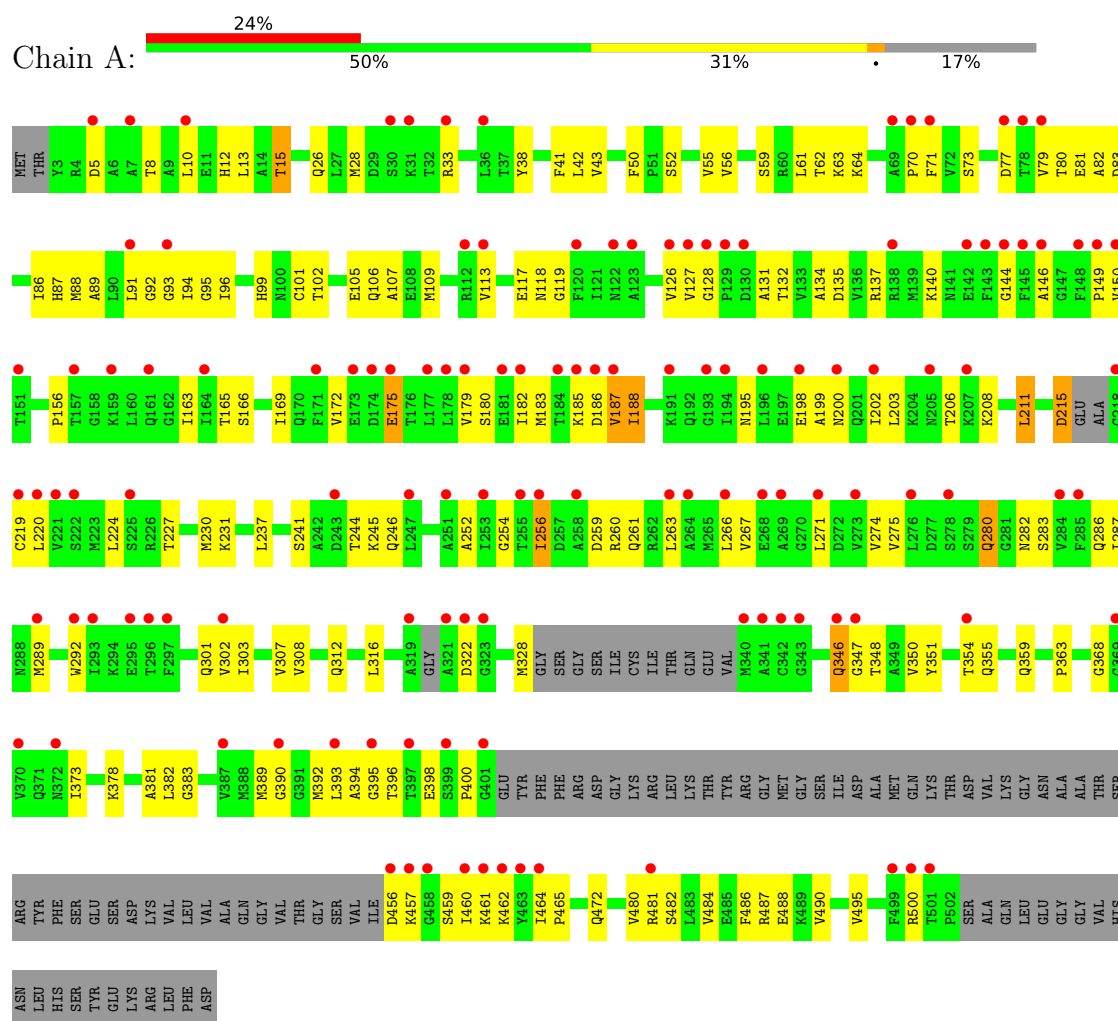
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total	O	0	0
			52	52		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	148.54Å 148.54Å 103.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.10 – 2.11 85.10 – 2.11	Depositor EDS
% Data completeness (in resolution range)	66.4 (85.10-2.11) 66.7 (85.10-2.11)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.15rc1_3420: ???)	Depositor
R, R_{free}	0.254 , 0.283 0.273 , 0.288	Depositor DCC
R_{free} test set	1090 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6538	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: G5P, GDP, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.98	1/3215 (0.0%)	1.55	6/4351 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	MET	C-O	-7.33	1.15	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ILE	CA-C-N	5.42	127.54	120.28
1	A	256	ILE	C-N-CA	5.42	127.54	120.28
1	A	52	SER	CA-C-N	5.31	127.39	120.28
1	A	52	SER	C-N-CA	5.31	127.39	120.28
1	A	208	LYS	CA-C-N	5.23	125.75	120.00
1	A	208	LYS	C-N-CA	5.23	125.75	120.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3171	3165	3157	198	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	58	24	24	8	0
3	A	28	12	12	3	0
4	A	16	12	12	1	0
5	A	52	0	0	3	0
All	All	3325	3213	3205	198	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG21	1:A:183:MET:CE	1.32	1.56
1:A:150:VAL:CG2	1:A:183:MET:CE	2.10	1.27
1:A:150:VAL:CB	1:A:183:MET:HE1	1.69	1.22
1:A:150:VAL:CG2	1:A:183:MET:HE2	1.70	1.21
1:A:200:ASN:OD1	3:A:602:GDP:O2'	1.58	1.19
1:A:350:VAL:O	1:A:354:THR:OG1	1.68	1.10
1:A:89:ALA:HA	1:A:93:GLY:O	1.58	1.03
1:A:134:ALA:HB2	1:A:175:GLU:HG3	1.43	1.01
1:A:302:VAL:N	1:A:322:ASP:OD2	1.93	0.99
1:A:150:VAL:CG1	1:A:183:MET:HE1	1.93	0.96
1:A:150:VAL:HB	1:A:183:MET:HE1	1.47	0.95
1:A:150:VAL:HG21	1:A:183:MET:HE2	0.93	0.93
1:A:99:HIS:HB3	1:A:252:ALA:O	1.69	0.92
1:A:73:SER:OG	1:A:95:GLY:HA2	1.71	0.91
1:A:150:VAL:HG21	1:A:183:MET:HE3	1.51	0.90
1:A:5:ASP:O	1:A:8:THR:HG22	1.70	0.89
1:A:260:ARG:HH12	1:A:292:TRP:CG	1.91	0.88
1:A:283:SER:O	1:A:287:ILE:HG13	1.75	0.87
1:A:150:VAL:HG11	1:A:183:MET:HE1	1.57	0.86
1:A:59:SER:OG	1:A:70:PRO:HB3	1.77	0.85
1:A:102:THR:OG1	1:A:105:GLU:HG3	1.76	0.85
1:A:5:ASP:O	1:A:8:THR:CG2	2.25	0.84
1:A:140:LYS:HD2	1:A:146:ALA:HB2	1.61	0.83
1:A:165:THR:HB	2:A:601:G5P:O2D	1.79	0.82
1:A:91:LEU:HD13	1:A:464:ILE:HB	1.62	0.82
1:A:187:VAL:HA	2:A:601:G5P:C2A	2.10	0.81
1:A:150:VAL:HG11	1:A:183:MET:CE	2.10	0.81
1:A:231:LYS:NZ	5:A:702:HOH:O	2.14	0.81
1:A:195:ASN:OD1	1:A:198:GLU:CB	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:CB	1:A:183:MET:CE	2.45	0.80
1:A:199:ALA:HB1	1:A:224:LEU:CD1	2.12	0.79
1:A:461:LYS:O	1:A:465:PRO:HG2	1.83	0.79
1:A:86:ILE:HG13	1:A:113:VAL:HG22	1.65	0.78
1:A:215:ASP:OD2	1:A:219:CYS:HB2	1.85	0.77
1:A:394:ALA:O	1:A:457:LYS:HE2	1.86	0.76
1:A:398:GLU:OE2	1:A:459:SER:OG	2.05	0.75
1:A:461:LYS:O	1:A:465:PRO:CG	2.35	0.75
1:A:169:ILE:HA	1:A:172:VAL:CG2	2.17	0.74
1:A:89:ALA:CA	1:A:93:GLY:O	2.35	0.74
1:A:203:LEU:O	1:A:203:LEU:HD23	1.88	0.73
1:A:102:THR:OG1	1:A:105:GLU:CG	2.36	0.72
1:A:256:ILE:HG12	1:A:259:ASP:OD2	1.89	0.72
1:A:156:PRO:O	1:A:220:LEU:HD23	1.90	0.71
1:A:199:ALA:HB1	1:A:224:LEU:HD11	1.72	0.70
1:A:107:ALA:HA	1:A:266:LEU:HD23	1.73	0.70
1:A:398:GLU:OE1	1:A:398:GLU:N	2.23	0.70
1:A:307:VAL:CG1	1:A:316:LEU:HD12	2.22	0.69
1:A:260:ARG:NH1	1:A:292:TRP:CG	2.60	0.69
1:A:102:THR:HG1	1:A:105:GLU:CD	2.00	0.69
1:A:119:GLY:O	1:A:224:LEU:CD2	2.41	0.68
1:A:308:VAL:HG11	1:A:328:MET:HB3	1.75	0.68
1:A:102:THR:HG1	1:A:105:GLU:CG	2.07	0.67
1:A:211:LEU:HB3	1:A:224:LEU:HB2	1.77	0.67
1:A:73:SER:OG	1:A:95:GLY:CA	2.42	0.66
1:A:102:THR:OG1	1:A:105:GLU:CD	2.40	0.65
1:A:169:ILE:HA	1:A:172:VAL:HG23	1.79	0.64
1:A:282:ASN:HB2	1:A:312:GLN:HG2	1.80	0.64
1:A:227:THR:OG1	2:A:601:G5P:O2A	2.14	0.64
1:A:195:ASN:OD1	1:A:198:GLU:N	2.27	0.64
1:A:62:THR:CB	1:A:301:GLN:HE21	2.11	0.64
1:A:307:VAL:HG11	1:A:316:LEU:HD12	1.81	0.63
1:A:462:LYS:C	1:A:465:PRO:HD2	2.22	0.63
1:A:187:VAL:HA	2:A:601:G5P:H6	1.80	0.63
1:A:392:MET:O	1:A:457:LYS:HD2	1.98	0.63
1:A:87:HIS:CB	1:A:460:ILE:HD11	2.28	0.63
1:A:373:ILE:H	1:A:373:ILE:HD12	1.64	0.62
1:A:56:VAL:CG2	1:A:482:SER:CB	2.78	0.62
1:A:132:THR:CG2	1:A:135:ASP:CG	2.73	0.62
1:A:71:PHE:HB3	1:A:389:MET:CE	2.31	0.61
1:A:12:HIS:O	1:A:15:THR:HB	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:CG1	1:A:183:MET:CE	2.67	0.60
1:A:137:ARG:HG3	1:A:169:ILE:HD12	1.84	0.60
1:A:203:LEU:HA	1:A:206:THR:CG2	2.31	0.60
1:A:254:GLY:HA3	1:A:259:ASP:OD2	2.02	0.60
1:A:169:ILE:HA	1:A:172:VAL:HG21	1.83	0.60
1:A:102:THR:OG1	1:A:105:GLU:OE1	2.20	0.59
1:A:119:GLY:O	1:A:224:LEU:HD23	2.02	0.59
1:A:274:VAL:CG1	1:A:302:VAL:HG22	2.32	0.59
1:A:87:HIS:HB3	1:A:460:ILE:HD11	1.84	0.59
1:A:79:VAL:CG2	1:A:390:GLY:O	2.52	0.58
1:A:180:SER:HA	1:A:183:MET:HG2	1.85	0.58
1:A:199:ALA:CB	1:A:224:LEU:HD11	2.34	0.58
1:A:56:VAL:CG2	1:A:482:SER:HB3	2.35	0.57
1:A:92:GLY:HA2	1:A:237:LEU:O	2.05	0.57
1:A:56:VAL:HG23	1:A:482:SER:HB2	1.86	0.57
1:A:302:VAL:O	1:A:322:ASP:HB2	2.04	0.57
1:A:188:ILE:N	2:A:601:G5P:N1A	2.48	0.57
1:A:140:LYS:CD	1:A:146:ALA:HB2	2.33	0.57
1:A:188:ILE:N	1:A:188:ILE:HD12	2.19	0.57
1:A:165:THR:OG1	2:A:601:G5P:H3'	2.05	0.57
1:A:203:LEU:HA	1:A:206:THR:HG22	1.87	0.57
1:A:241:SER:N	1:A:246:GLN:O	2.34	0.56
1:A:393:LEU:O	1:A:396:THR:OG1	2.21	0.56
1:A:301:GLN:HA	1:A:322:ASP:OD2	2.05	0.56
1:A:26:GLN:O	1:A:33:ARG:NH2	2.35	0.55
1:A:203:LEU:HD23	1:A:203:LEU:C	2.32	0.55
1:A:79:VAL:HG21	1:A:390:GLY:O	2.06	0.55
1:A:346:GLN:HA	1:A:346:GLN:OE1	2.06	0.55
1:A:128:GLY:O	1:A:179:VAL:HG21	2.07	0.55
1:A:260:ARG:NH1	1:A:292:TRP:CD2	2.75	0.54
1:A:80:THR:HG21	1:A:96:ILE:O	2.08	0.54
1:A:275:VAL:HG22	1:A:303:ILE:HB	1.90	0.54
1:A:146:ALA:HB3	1:A:166:SER:OG	2.08	0.53
1:A:59:SER:CB	1:A:70:PRO:HB3	2.37	0.53
1:A:55:VAL:O	1:A:472:GLN:NE2	2.40	0.53
1:A:140:LYS:O	1:A:144:GLY:N	2.41	0.52
1:A:260:ARG:HH12	1:A:292:TRP:CD1	2.25	0.52
1:A:5:ASP:O	1:A:8:THR:HG23	2.07	0.52
1:A:132:THR:HG22	1:A:135:ASP:CG	2.34	0.52
1:A:461:LYS:O	1:A:465:PRO:CD	2.58	0.52
1:A:71:PHE:HB3	1:A:389:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:N	1:A:10:LEU:CD1	2.73	0.52
1:A:484:VAL:O	1:A:488:GLU:HG3	2.10	0.51
1:A:179:VAL:O	1:A:183:MET:N	2.43	0.51
1:A:462:LYS:O	1:A:465:PRO:HD2	2.11	0.51
1:A:203:LEU:CA	1:A:206:THR:HG22	2.42	0.50
1:A:56:VAL:HG22	1:A:482:SER:HB3	1.92	0.50
1:A:10:LEU:N	1:A:10:LEU:HD12	2.27	0.50
1:A:132:THR:HG23	1:A:135:ASP:H	1.77	0.50
1:A:77:ASP:O	1:A:400:PRO:HG3	2.12	0.49
1:A:82:ALA:HB3	5:A:731:HOH:O	2.12	0.49
1:A:55:VAL:HA	1:A:481:ARG:O	2.12	0.49
1:A:187:VAL:HA	2:A:601:G5P:N1A	2.26	0.49
1:A:42:LEU:HD11	1:A:500:ARG:HD3	1.93	0.49
1:A:71:PHE:HB3	1:A:389:MET:HE2	1.94	0.49
1:A:88:MET:O	1:A:93:GLY:O	2.31	0.49
1:A:150:VAL:HG11	1:A:183:MET:HE3	1.91	0.49
1:A:62:THR:C	1:A:363:PRO:HG3	2.37	0.49
1:A:203:LEU:C	1:A:203:LEU:CD2	2.85	0.49
1:A:282:ASN:CB	1:A:312:GLN:HG2	2.42	0.48
1:A:480:VAL:HG11	1:A:486:PHE:HA	1.95	0.48
1:A:56:VAL:CG2	1:A:482:SER:HB2	2.44	0.48
1:A:107:ALA:HA	1:A:266:LEU:CD2	2.42	0.48
1:A:56:VAL:HG23	1:A:482:SER:CB	2.43	0.48
1:A:464:ILE:N	1:A:465:PRO:CD	2.77	0.48
1:A:165:THR:CB	2:A:601:G5P:O2D	2.55	0.48
1:A:202:ILE:O	1:A:206:THR:HG22	2.14	0.48
1:A:241:SER:O	1:A:245:LYS:N	2.44	0.47
1:A:81:GLU:HA	1:A:109:MET:CE	2.44	0.47
1:A:211:LEU:C	1:A:211:LEU:HD13	2.39	0.47
1:A:64:LYS:HB2	1:A:301:GLN:CD	2.39	0.47
1:A:88:MET:C	1:A:93:GLY:O	2.57	0.47
1:A:117:GLU:OE2	3:A:602:GDP:O6	2.33	0.47
1:A:231:LYS:CE	5:A:702:HOH:O	2.61	0.46
1:A:261:GLN:NE2	1:A:261:GLN:HA	2.30	0.46
1:A:260:ARG:NH1	1:A:292:TRP:CD1	2.84	0.46
1:A:10:LEU:O	1:A:13:LEU:HB3	2.16	0.46
1:A:119:GLY:HA2	3:A:602:GDP:C2	2.51	0.46
1:A:302:VAL:H	1:A:322:ASP:CG	2.08	0.46
1:A:80:THR:HG21	1:A:96:ILE:C	2.41	0.46
1:A:263:LEU:O	1:A:267:VAL:HG23	2.15	0.46
1:A:383:GLY:HA2	1:A:487:ARG:CZ	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:N	1:A:188:ILE:CD1	2.78	0.45
1:A:280:GLN:OE1	1:A:312:GLN:NE2	2.49	0.45
1:A:199:ALA:CB	1:A:224:LEU:CD1	2.91	0.45
1:A:101:CYS:SG	1:A:106:GLN:HB2	2.56	0.45
1:A:203:LEU:C	1:A:206:THR:HG22	2.41	0.45
1:A:87:HIS:HB2	1:A:460:ILE:HD11	1.98	0.45
1:A:118:ASN:ND2	1:A:246:GLN:OE1	2.47	0.45
1:A:127:VAL:HG22	1:A:131:ALA:CB	2.47	0.44
1:A:42:LEU:CD1	1:A:500:ARG:HB2	2.48	0.44
1:A:131:ALA:O	1:A:179:VAL:HG13	2.18	0.44
1:A:182:ILE:O	1:A:182:ILE:HG22	2.18	0.44
1:A:81:GLU:HA	1:A:109:MET:HE1	2.00	0.44
1:A:180:SER:CA	1:A:183:MET:HG2	2.46	0.44
1:A:28:MET:CE	1:A:348:THR:HA	2.49	0.43
1:A:82:ALA:O	1:A:86:ILE:HG13	2.19	0.43
1:A:351:TYR:O	1:A:355:GLN:HB2	2.18	0.43
1:A:62:THR:HB	1:A:301:GLN:HE21	1.84	0.43
1:A:183:MET:O	1:A:183:MET:HG3	2.19	0.43
1:A:254:GLY:CA	1:A:259:ASP:OD2	2.66	0.43
1:A:83:ASP:OD1	1:A:87:HIS:CE1	2.72	0.43
1:A:266:LEU:HB3	1:A:271:LEU:HD22	2.01	0.43
1:A:392:MET:O	1:A:457:LYS:CD	2.67	0.43
1:A:91:LEU:HD11	1:A:461:LYS:HA	2.00	0.42
1:A:50:PHE:CG	1:A:481:ARG:HG2	2.54	0.42
1:A:137:ARG:NH2	1:A:169:ILE:O	2.53	0.42
1:A:132:THR:HG23	1:A:135:ASP:CG	2.44	0.42
1:A:28:MET:HE2	1:A:348:THR:HA	2.01	0.42
1:A:149:PRO:HA	1:A:163:ILE:HA	2.00	0.42
1:A:347:GLY:O	1:A:382:LEU:HD13	2.19	0.42
1:A:490:VAL:HA	1:A:495:VAL:HB	2.02	0.42
1:A:38:TYR:O	1:A:378:LYS:HD3	2.20	0.42
1:A:62:THR:OG1	1:A:301:GLN:NE2	2.43	0.42
1:A:381:ALA:O	1:A:490:VAL:HG11	2.20	0.42
1:A:126:VAL:HG12	1:A:149:PRO:HG2	2.01	0.41
1:A:368:GLY:HA2	4:A:603:ACT:H2	2.01	0.41
1:A:381:ALA:HB2	1:A:486:PHE:CZ	2.55	0.41
1:A:244:THR:O	1:A:245:LYS:HB2	2.21	0.41
1:A:61:LEU:HD22	1:A:94:ILE:HG21	2.01	0.41
1:A:230:MET:HE2	1:A:230:MET:HB3	1.96	0.41
1:A:308:VAL:HG11	1:A:328:MET:CB	2.49	0.41
1:A:134:ALA:HB2	1:A:175:GLU:CG	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:O	1:A:206:THR:HG22	2.20	0.40
1:A:211:LEU:C	1:A:211:LEU:CD1	2.94	0.40
1:A:203:LEU:O	1:A:206:THR:CG2	2.69	0.40
1:A:395:GLY:O	1:A:456:ASP:HA	2.21	0.40
1:A:41:PHE:O	1:A:378:LYS:NZ	2.52	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:CG	1:A:186:ASP:CB[6_546]	1.56	0.64
1:A:185:LYS:HG3	1:A:186:ASP:CB[6_546]	1.00	0.60
1:A:12:HIS:HE2	1:A:359:GLN:HE22[4_555]	1.32	0.28

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	422/522 (81%)	417 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/429 (77%)	318 (97%)	11 (3%)	33	36

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	43	VAL
1	A	63	LYS
1	A	175	GLU
1	A	187	VAL
1	A	188	ILE
1	A	211	LEU
1	A	215	ASP
1	A	280	GLN
1	A	286	GLN
1	A	346	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	99	HIS
1	A	100	ASN
1	A	205	ASN
1	A	233	GLN
1	A	261	GLN
1	A	301	GLN
1	A	359	GLN
1	A	469	ASN
1	A	473	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	A	603	-	3,3,3	0.74	0	3,3,3	1.79	2 (66%)
2	G5P	A	601	-	63,63,63	1.23	8 (12%)	91,100,100	1.80	17 (18%)
4	ACT	A	606	-	3,3,3	0.99	0	3,3,3	1.52	1 (33%)
4	ACT	A	605	-	3,3,3	0.77	0	3,3,3	1.81	2 (66%)
3	GDP	A	602	-	29,30,30	1.14	3 (10%)	45,47,47	1.82	7 (15%)
4	ACT	A	604	-	3,3,3	0.59	0	3,3,3	1.85	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	A	602	-	-	2/16/32/32	0/3/3/3
2	G5P	A	601	-	-	8/44/76/76	0/6/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	G5P	C5A-C4A	4.24	1.46	1.39
3	A	602	GDP	C5-C4	2.94	1.46	1.38
2	A	601	G5P	C5-C4	2.88	1.46	1.38
2	A	601	G5P	C5A-C6A	2.59	1.48	1.41
2	A	601	G5P	C6-N1	-2.58	1.34	1.38
3	A	602	GDP	C6-N1	-2.51	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	G5P	C5A-N7A	-2.49	1.34	1.39
2	A	601	G5P	C5-N7	-2.38	1.34	1.39
2	A	601	G5P	C4A-N9A	-2.21	1.33	1.37
3	A	602	GDP	C5-N7	-2.20	1.34	1.39
2	A	601	G5P	C8A-N7A	2.06	1.35	1.31

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	G5P	C5-C4-N3	-6.23	118.47	128.39
3	A	602	GDP	C5-C4-N3	-6.15	118.60	128.39
2	A	601	G5P	C5A-C4A-N3A	-5.67	118.91	126.72
3	A	602	GDP	C2-N3-C4	5.00	120.92	112.30
2	A	601	G5P	C2-N3-C4	5.00	120.91	112.30
2	A	601	G5P	N9-C4-N3	4.72	135.39	125.95
3	A	602	GDP	N9-C4-N3	4.65	135.26	125.95
2	A	601	G5P	N3A-C4A-N9A	4.57	134.94	127.17
2	A	601	G5P	C2A-N3A-C4A	3.85	121.24	111.83
2	A	601	G5P	N1A-C2A-N3A	-3.74	122.92	128.58
2	A	601	G5P	C4A-C5A-N7A	-3.63	106.44	110.58
2	A	601	G5P	C4A-N9A-C8A	3.25	109.15	105.74
3	A	602	GDP	C6-C5-N7	3.17	136.05	130.29
2	A	601	G5P	C6-C5-N7	3.10	135.92	130.29
2	A	601	G5P	C5A-N7A-C8A	2.83	107.90	103.45
2	A	601	G5P	C4-C5-N7	-2.60	106.54	110.67
3	A	602	GDP	C4-C5-N7	-2.56	106.62	110.67
2	A	601	G5P	N9A-C8A-N7A	-2.52	110.36	113.94
3	A	602	GDP	C3'-C2'-C1'	2.29	105.80	101.46
2	A	601	G5P	C6A-C5A-N7A	2.29	136.50	132.09
4	A	604	ACT	O-C-CH3	-2.27	113.21	122.53
4	A	605	ACT	O-C-CH3	-2.26	113.24	122.53
3	A	602	GDP	O6-C6-C5	-2.26	120.56	126.53
4	A	604	ACT	OXT-C-O	2.22	130.27	122.03
4	A	603	ACT	O-C-CH3	-2.22	113.43	122.53
2	A	601	G5P	C2A-N1A-C6A	2.17	122.30	118.73
2	A	601	G5P	O6-C6-C5	-2.16	120.84	126.53
4	A	606	ACT	OXT-C-O	2.15	130.02	122.03
4	A	605	ACT	OXT-C-O	2.14	129.96	122.03
4	A	603	ACT	OXT-C-O	2.13	129.91	122.03
2	A	601	G5P	C8-N7-C5	2.03	107.87	104.26

There are no chirality outliers.

All (10) torsion outliers are listed below:

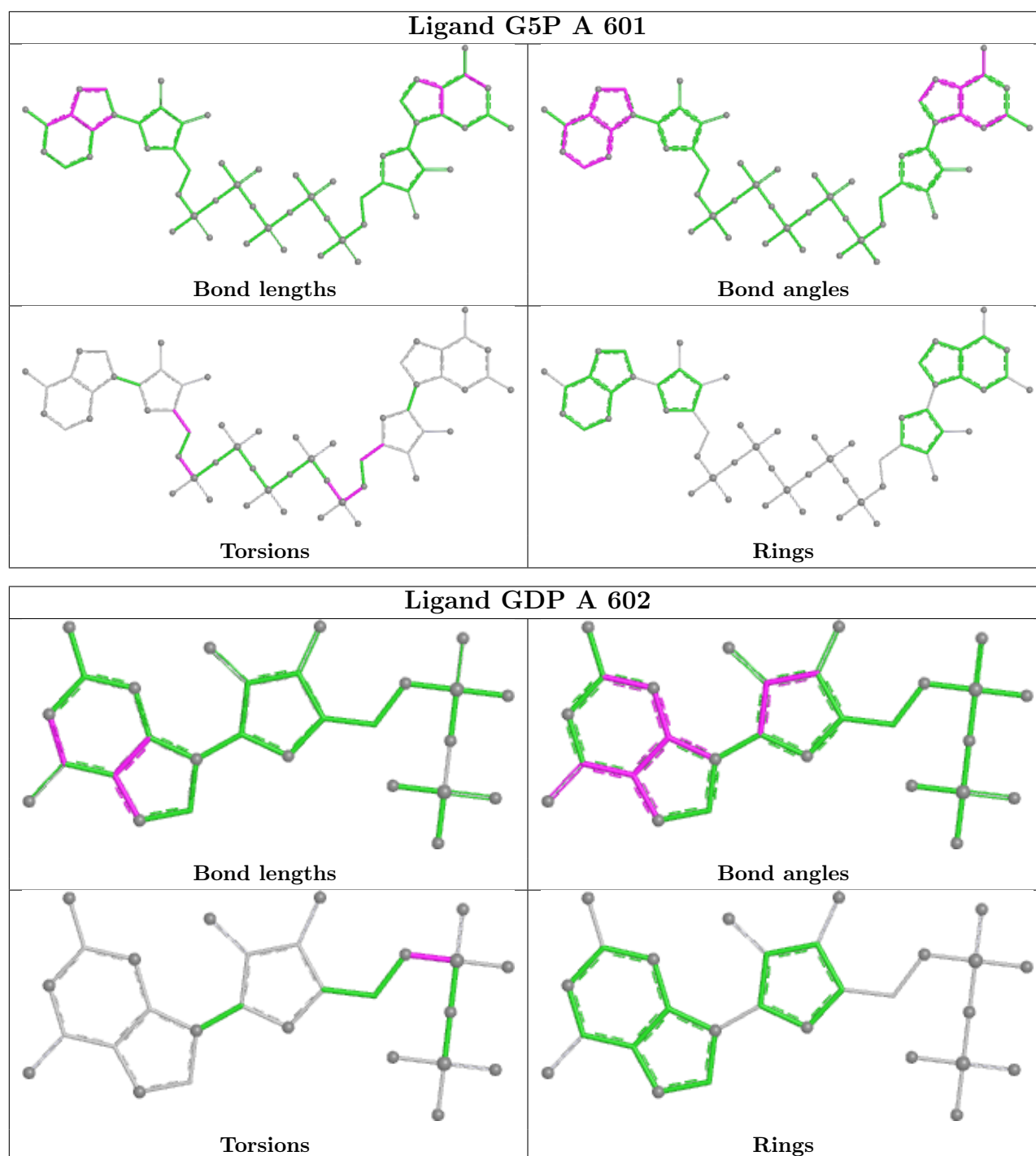
Mol	Chain	Res	Type	Atoms
2	A	601	G5P	C5F-O5F-PE-O1E
3	A	602	GDP	C5'-O5'-PA-O3A
2	A	601	G5P	O4'-C4'-C5'-O5'
2	A	601	G5P	C3'-C4'-C5'-O5'
2	A	601	G5P	O4F-C4F-C5F-O5F
2	A	601	G5P	C3F-C4F-C5F-O5F
2	A	601	G5P	C5F-O5F-PE-O3D
2	A	601	G5P	C5'-O5'-PA-O1A
3	A	602	GDP	C5'-O5'-PA-O1A
2	A	601	G5P	PB-O3A-PA-O1A

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	ACT	1	0
2	A	601	G5P	8	0
3	A	602	GDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	432/522 (82%)	1.59	125 (28%) 1 1	38, 66, 93, 121	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	ALA	6.4
1	A	243	ASP	6.3
1	A	390	GLY	6.0
1	A	218	GLY	5.8
1	A	184	THR	5.6
1	A	146	ALA	4.5
1	A	341	ALA	4.4
1	A	186	ASP	4.2
1	A	268	GLU	4.2
1	A	123	ALA	4.2
1	A	93	GLY	4.1
1	A	460	ILE	3.9
1	A	258	ALA	3.9
1	A	221	VAL	3.8
1	A	185	LYS	3.8
1	A	194	ILE	3.6
1	A	271	LEU	3.6
1	A	273	VAL	3.6
1	A	145	PHE	3.6
1	A	253	ILE	3.5
1	A	395	GLY	3.5
1	A	343	GLY	3.4
1	A	322	ASP	3.4
1	A	78	THR	3.3
1	A	340	MET	3.3
1	A	193	GLY	3.3
1	A	457	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	220	LEU	3.3
1	A	393	LEU	3.2
1	A	222	SER	3.2
1	A	181	GLU	3.1
1	A	464	ILE	3.1
1	A	143	PHE	3.1
1	A	200	ASN	3.1
1	A	285	PHE	3.1
1	A	7	ALA	3.0
1	A	370	VAL	3.0
1	A	36	LEU	3.0
1	A	142	GLU	3.0
1	A	342	CYS	2.9
1	A	130	ASP	2.9
1	A	148	PHE	2.9
1	A	456	ASP	2.9
1	A	157	THR	2.8
1	A	171	PHE	2.8
1	A	499	PHE	2.8
1	A	463	TYR	2.8
1	A	77	ASP	2.8
1	A	198	GLU	2.7
1	A	354	THR	2.7
1	A	187	VAL	2.7
1	A	128	GLY	2.7
1	A	500	ARG	2.7
1	A	173	GLU	2.6
1	A	397	THR	2.6
1	A	501	THR	2.6
1	A	31	LYS	2.6
1	A	461	LYS	2.6
1	A	219	CYS	2.6
1	A	297	PHE	2.6
1	A	399	SER	2.6
1	A	202	ILE	2.5
1	A	178	LEU	2.5
1	A	292	TRP	2.5
1	A	179	VAL	2.5
1	A	122	ASN	2.5
1	A	10	LEU	2.5
1	A	33	ARG	2.5
1	A	71	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	144	GLY	2.5
1	A	129	PRO	2.4
1	A	138	ARG	2.4
1	A	481	ARG	2.4
1	A	293	ILE	2.4
1	A	296	THR	2.4
1	A	401	GLY	2.4
1	A	79	VAL	2.4
1	A	91	LEU	2.4
1	A	302	VAL	2.4
1	A	276	LEU	2.3
1	A	347	GLY	2.3
1	A	346	GLN	2.3
1	A	255	THR	2.3
1	A	196	LEU	2.3
1	A	159	LYS	2.3
1	A	191	LYS	2.3
1	A	150	VAL	2.3
1	A	369	GLY	2.3
1	A	247	LEU	2.3
1	A	225	SER	2.2
1	A	458	GLY	2.2
1	A	263	LEU	2.2
1	A	266	LEU	2.2
1	A	70	PRO	2.2
1	A	164	ILE	2.2
1	A	127	VAL	2.2
1	A	319	ALA	2.2
1	A	161	GLN	2.2
1	A	207	LYS	2.2
1	A	205	ASN	2.2
1	A	120	PHE	2.2
1	A	151	THR	2.2
1	A	5	ASP	2.2
1	A	256	ILE	2.2
1	A	295	GLU	2.2
1	A	323	GLY	2.2
1	A	251	ALA	2.2
1	A	269	ALA	2.2
1	A	177	LEU	2.2
1	A	289	MET	2.2
1	A	175	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	387	VAL	2.1
1	A	174	ASP	2.1
1	A	113	VAL	2.1
1	A	284	VAL	2.1
1	A	149	PRO	2.1
1	A	126	VAL	2.1
1	A	30	SER	2.1
1	A	112	ARG	2.1
1	A	182	ILE	2.1
1	A	264	ALA	2.1
1	A	278	SER	2.1
1	A	372	ASN	2.0
1	A	69	ALA	2.0
1	A	462	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

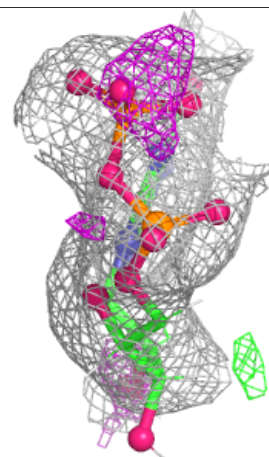
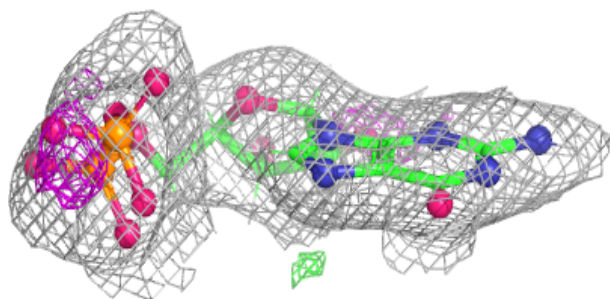
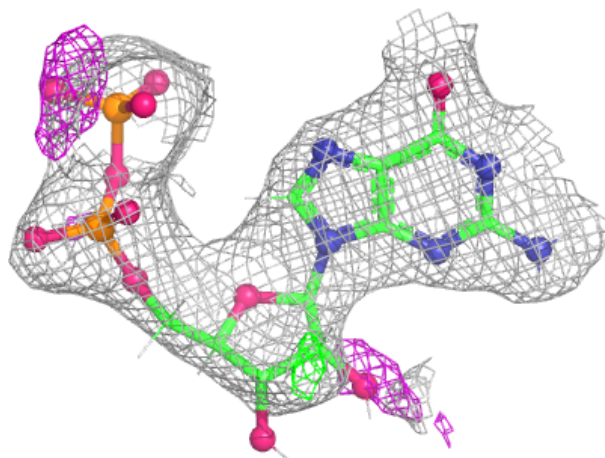
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	605	4/4	0.47	0.16	73,73,90,90	0
4	ACT	A	606	4/4	0.64	0.15	63,63,78,78	0
3	GDP	A	602	28/28	0.78	0.13	67,81,101,101	0
4	ACT	A	603	4/4	0.82	0.20	43,44,54,54	0
4	ACT	A	604	4/4	0.82	0.14	58,58,71,71	0
2	G5P	A	601	58/58	0.88	0.11	43,60,72,78	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

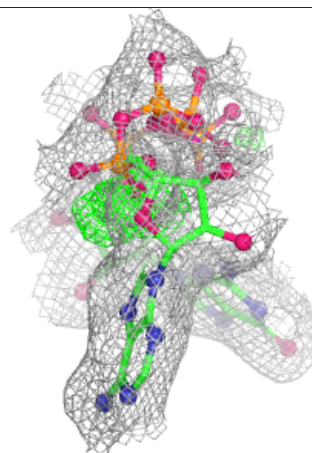
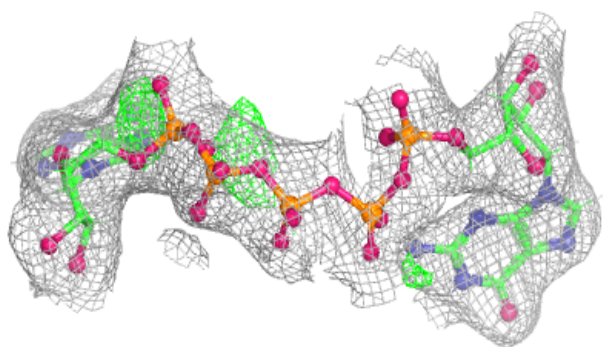
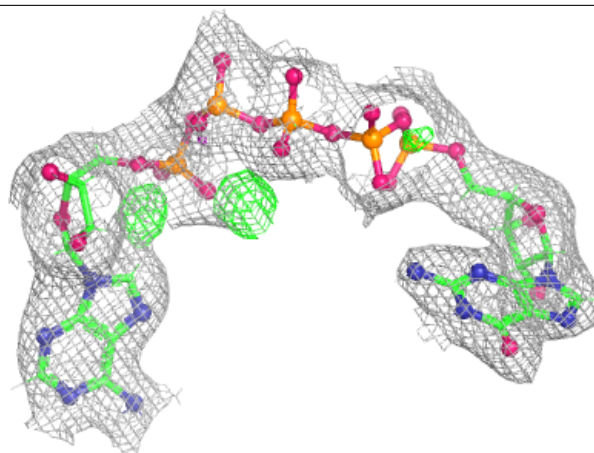
Electron density around GDP A 602:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G5P A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.